3rd Annual CCP13/NCD Workshop

The third annual workshop for the collaborative computational project for fibre diffraction (CCP13) was held in the Tower block seminar room at Daresbury from May 9-11, 1994. This year the meeting was combined with the non-crystalline diffraction (NCD) specialist user group and attracted over 80 participants, twice the number who attended the previous two workshops and reflecting the interest shown in the field. The meeting was partially sponsored by Molecular Simulations and BioSym.

To reflect the joint nature of the workshop a new programme format was devised covering a diversity of topics, including synthetic polymers and liquid crystals, hardware sources and detectors, software developments and biological systems. Each session began with an eminent keynote speaker followed by presentations from specialists in the field. Extending our policy of forging international links, speakers from Australia, France, Austria, Germany and the USA, were invited to give presentations. The talks were complemented by a poster session and commercial exhibition (BioSym and Sun Microsystems).

The meeting opened with a lively presentation by the keynote speaker for the polymer session O.Glatter (Graz), on the desmearing of low angle diffraction patterns, using cubic slines, to reduce the effect of slit width. This was followed by talks from W.Bras (Daresbury) on the combination of simultaneous time resolved techniques small with wide angle scattering (SAX/WAX), including differential scanning calorimetry and Fourier Transform Infra Red. M.J.Elwell (UMIST) described the use of SAX to study the kinetics of flexible polyurethane foam and R.J.Rule (ICI) presented a study on oriented synthetic polymers with a paracrystalline macrolattice. H.F.Gleeson (Manchester) described the application of time resolved X-Ray scattering to the study liquid crystals in the Smectic A phase. A.Mahendrasingham (Keele) described the results of fibre diffraction studies of the structural transitions in organic polymers and the development of a new CCD detector system. A.J.Ryan (UMIST) concluded with a talk on SAX/WAX studies on the polymorphism of polybut-1-ene explaining why bin-bag liners are black.

The hardware session started with C.Reikel (ESRF) providing a description of the facilities at the ESRF for SAX and polymers under high pressure. This was followed by C.C.Wilson (Rutherford Appleton) who described the use of neutron time of flight Laue diffraction and its application to fibres. G.Hall (Imperial College) gave a technical presentation on future detectors constructed from silicon with embedded electronics. N.Fore (Daresbury) described the necessary error corrections that would be required by the new generation of wire chamber detectors. This session was concluded with an overview of the facilities provided by the new Wiggler II station 16.1 on the SRS by E.Towns-Andrews (Daresbury) and the latest improvements in the stopped flow apparatus for studying fast kinetics using time resolved X-Ray diffraction by D.Clarke (Daresbury).

The software developments and results section began with a keynote address on the analysis and simulation of fibre diffraction patterns, emphasing the benefits of converting intensities into a reciprocal space map, by R.D.B.Fraser (Queensland). A.Windle (Cambridge) presented the development of a novel CCD based diffractometer, utilising a three circle goniometer, developed for oriented polymer fibres. The technique relies on the combination of images converted to reciprocal space. D.Svergun (EMBL) described a new approach to interpretation of small angle scattering data to provide shape determination as applied to the 50S ribosomal subunit, using spherical harmonics. W.J.Stroud (Purdue) described the effect of disorder in the crystalline domains of fibres on layer line intensities, showing that there is a gradual transition from Bragg to continuous intensity away from the centre of calculated patterns. A.P.Hammersley (ESRF) described some new developments in a 2D polynomial fitting background subtraction program and its application to the analysis of type I collagen. R.C.Denny (Imperial College & Daresbury) provided an overview of the CCP13 suite of programs including new developments in the LSQINT program with a maximum entropy algorithm. The final presentation of the session was given by A.Stewart (Kings College) who demonstated with a visual presentation the PC

software used to analyse muscle data recorded at CHESS.

The fourth session on biological systems commenced, with a second presentation by R.D.B.fraser (Queensland), with a review of the molecular structure and cellular organisation of keratin with special emphasis on the outstanding problems in this and collagen. T.Wess (Edinburgh) described modelling the three dimensional structure of type I collagen, both native and heavy atom labelled, to a triclinic unit cell. and K.M.Meek (Open University) showed how the collagen fibrils in scar tissue, from corneal stroma, becomes more ordered but never achieves a normal ordering.

K.C.Holmes (Heidelburg) lead a group of talks on muscle research by describing the structure of F-actin and myosin S1 determined by a combination of protein crystallography and X-Ray fibre diffraction techniques. He also addressed the nature of the actomyosin complex in rigor, by combining the results of cryo-electron microscopy and the crystallographic structures. L.C.Yu (NIH Bethesda) discussed recent results from X-Ray diffraction studies of myosin layer lines in skinned rabbit psoas muscle fibres to determine the effect of temperature and ionic strength on weakly bound cross bridges. Despite a wide variation in the number of attached cross bridges her results showed demonstrated that this did not disrupt the thick filament based arrangement of cross bridges in relaxed muscle. J.M.Squire (Imperial College) described recent developments in the analysis of X-Ray diffraction patterns from fish muscle. By utilising the CCP13 suite of programs, he has made significant progress in modelling the rest state at low resolution, with an aim to modelling the intermediate states to the plateau of tension thereby creating "Muscle the movie".

Finally, V.T.Forsyth (Keele) described the use of X-Ray and neutron fibre diffraction in probing the conformational stability in DNA polymers. M.K.Behan-Martin (Daresbury) discussed the swelling properties and phase behaviour of pharmaceutical ionic and non-ionic creams. J.G.Grossman (Daresbury) described some results of X-Ray solution scattering and modelling on two metalloprotein families, nitrite reductase and transferrin.

B.Fraser and C.Reikel volunteered to be judges for the best poster prize. The First place prize, a cheque for £70, was presented to Ann Willoughby (University of Cambridge), for her poster on "A novel CCD-based polymer fibre X-Ray diffractometer", by chairman J.Squire. Second place was awarded to Mike Elwell along with a cheque for £30. The workshop concluded with a special vote of thanks to Brenda Hamblett for all the hard work and organisation that went into making the whole meeting run smoothly.

Geoff Mant (CCP13 Secretary) Daresbury.

IF YOU ARE A FIBRE DIFFRACTIONIST STUDYING SYNTHETIC OR BIOLOGICAL POLYMERS - THIS CCP IS FOR YOU - PLEASE HELP TO MAKE IT WORK!

Dr. Tony Ryan demonstrates, to 2 delegates during the poster/wine tasting session at the 3rd Annual workshop, the use of correlation functions in the analysis of time resolved small angle X-ray data.